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(CS) field  
NEWS 4 AUG 24 ENCOMPLIT/ENCOMPLIT2 reloaded and enhanced  
NEWS 5 AUG 24 CA/Caplus enhanced with legal status information for  
U.S. patents  
NEWS 6 SEP 09 50 Millionth Unique Chemical Substance Recorded in  
CAS REGISTRY  
NEWS 7 SEP 11 WPIDS, WPINDEX, and WPIX now include Japanese FTERM  
thesaurus

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FILE 'HOME' ENTERED AT 12:14:10 ON 06 OCT 2009

=> file reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.22	0.22

FILE 'REGISTRY' ENTERED AT 12:14:25 ON 06 OCT 2009

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STRUCTURE FILE UPDATES: 4 OCT 2009 HIGHEST RN 1187307-68-1  
DICTIONARY FILE UPDATES: 4 OCT 2009 HIGHEST RN 1187307-68-1

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TSCA INFORMATION NOW CURRENT THROUGH June 26, 2009.

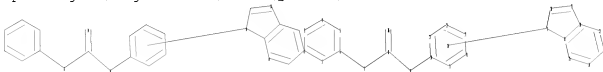
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chain nodes :
7 8 9 16
ring nodes :
1 2 3 4 5 6 10 11 12 13 14 15 17 18 19 20 21 22 23 24 25
chain bonds :
6-7 7-8 8-9 8-16 9-10
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15 17-18
17-21 18-19 19-20 20-21 20-22 21-25 22-23 23-24 24-25
exact/norm bonds :
6-7 7-8 8-9 8-16 9-10 17-18 17-21 18-19 19-20
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15 20-21
20-22 21-25 22-23 23-24 24-25
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Match level :

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1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom
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L1 STRUCTURE UPLOADED

=> s ll

SAMPLE SEARCH INITIATED 12:14:40 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 184 TO ITERATE

100.0% PROCESSED 184 ITERATIONS

8 ANSWERS

SEARCH TIME: 00.00.01

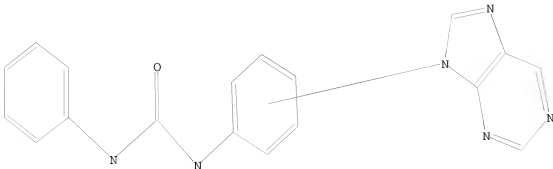
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BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 2867 TO 4493  
PROJECTED ANSWERS: 8 TO 329

L2 8 SEA SSS SAM L1

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L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam

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100.0% PROCESSED 184 ITERATIONS

8 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
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PROJECTED ITERATIONS: 2867 TO 4493  
PROJECTED ANSWERS: 8 TO 329

L3 8 SEA SSS SAM L1

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THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 185.40 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 12:15:00 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 3577 TO ITERATE

100.0% PROCESSED 3577 ITERATIONS

269 ANSWERS

SEARCH TIME: 00.00.01

L4 269 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

185.88

186.10

FILE 'CAPLUS' ENTERED AT 12:15:03 ON 06 OCT 2009

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FILE COVERS 1907 - 6 Oct 2009 VOL 151 ISS 15  
FILE LAST UPDATED: 5 Oct 2009 (20091005/ED)  
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Aug 2009  
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Aug 2009

CAPLUS now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2009.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l4

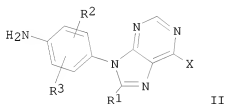
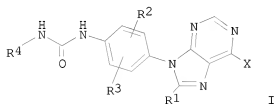
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L5 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 2006:1090595 CAPLUS  
DOCUMENT NUMBER: 145:438456  
TITLE: Preparation of purine derivatives as receptor-tyrosine kinase activity inhibitors  
INVENTOR(S): Hoelzemann, Guenter; Crassier, Helene; Rautenberg, Wilfried; Jonczyk, Alfred  
PATENT ASSIGNEE(S): Merck Patent GmbH, Germany  
SOURCE: PCT Int. Appl., 92pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006108482	A1	20061019	WO 2006-EP2380	20060315
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,			

GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,  
 KG, KZ, MD, RU, TJ, TM  
 DE 102005017259 A1 20061019 DE 2005-102005017259 20050414  
 AU 2006233530 A1 20061019 AU 2006-233530 20060315  
 CA 2604294 A1 20061019 CA 2006-2604294 20060315  
 EP 1869047 A1 20071226 EP 2006-723450 20060315  
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 JP 2008535874 T 20080904 JP 2008-505752 20060315  
 US 20080214582 A1 20080904 US 2008-910776 20080418  
 PRIORITY APPLN. INFO.: DE 2005-102005017259A 20050414  
 WO 2006-EP2380 W 20060315  
 OTHER SOURCE(S): CASREACT 145:438456  
 GI



AB The invention relates to compds. I [R1 = H, A; R2, R3 = H, A, Hal, OH, OA, CN; R4 = Ar, Het1; R5, R6 = H, A; X = OH, NH2; A = C1-10-alkyl, optionally substituted with 1 to 7 F or Cl; Ar = (un)substituted Ph optionally substituted with 1 to 3 from the following, Hal, A, OA, OH, C2-6-alkenyl, C2-6-alkynyl, NO2, NR5R6, C(=O)NR5R6, CO2H, CO2A, CN, CHO, COA, Ph, (CH2)nHet, O(CH2)nHet, NH(CH2)nHet, O(CH2)nCyc, N(CH2)nCyc, O(CH2)mNR5R6, NR1(CH2)mNR5R6, O(CH2)mNR10(CH2)mNR5R6; Het = (un)saturated or aromatic, mono- or bicyclic heterocycle containing 1 to 4 N, O and S and optionally substituted with 1 to 3 Hal, A, OA, Ph, CO2A, CN, CC(=O); Het1 = mono- or bicyclic, aromatic heterocycle containing 1 to 4 N, O and S and optionally substituted with 1 to 3 Hal, A, OA, OH, C2-6-alkenyl, C2-6-alkynyl, NO2, NR5R6, C(=O)NR5R6, CO2H, CO2A, CN, CHO, COA, Ph, (CH2)nHet, O(CH2)nHet, NH(CH2)nHet, O(CH2)nCyc, N(CH2)nCyc, O(CH2)mNR5R6, NR1(CH2)mNR5R6, O(CH2)mNR10(CH2)mNR5R6; Cyc = C3-7-cycloalkyl; Hal = F, Cl, Br, I; n = 0, 1, 2, 3, 4; m = 1, 2, 3, 4] or their pharmaceutically acceptable salts, solvates, tautomers, stereoisomers or their mixts., which are inhibitors of tyrosine kinases, in particular TIE-2, and the Raf-kinases and can be also be used for treating tumors. The procedure for the preparation of I comprises: carbamoylation of purinylanilines II with (a) isocyanates, R4NCO; or (b) carbamoylation by sequential addition of chloroformates

followed by amines R4NH2; or, (c) by solvolysis or hydrogenolysis of protected derivs. of II and its salts. Thus, 1-[4-(6-aminopurin-9-yl)phenyl]-3-[3-(trifluoromethyl)phenyl]urea [I; R1 = R2 = R3 = H; R4 = C6H4CF3-3; X = NH2] was prepd, from 9-(4-aminophenyl)adenine [II; R1 = R2 = R3 = H; X = NH2] via carbamoylation with 3-CF2C6H4NCO in CH2Cl2 containing Et3N. The enzyme inhibiting activity of I [R1 = R2 = R3 = H; R4 = C6H4CF3-3; X = NH2] was determined IC50 = 14 nmol/L vs. Tyrosine kinase receptor Tie-2 and IC50 = 3.6 nmol/L vs. Vascular endothelial growth factor receptors (VEGFR)].

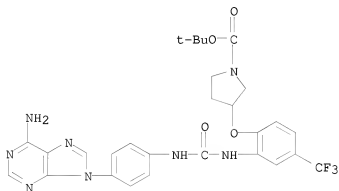
IT 912539-35-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and N-deprotection of; preparation of purine derivs. as receptor-tyrosine kinase activity inhibitors)

RN 912539-35-6 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 3-[2-[[[4-(6-amino-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-4-(trifluoromethyl)phenoxy]-, 1,1-dimethylethyl ester (CA INDEX NAME)



IT 912539-16-3P 912539-17-4P 912539-18-5P

912539-19-6P 912539-20-9P 912539-22-1P

912539-23-2P 912539-24-3P 912539-25-4P

912539-26-5P 912539-27-6P 912539-29-8P

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912539-44-7P 912539-45-8P 912539-46-9P

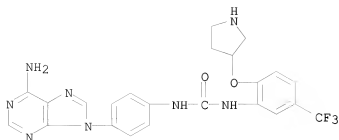
912539-48-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of purine derivs. as receptor-tyrosine kinase activity inhibitors)

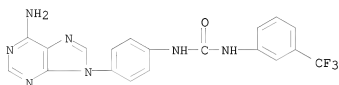
RN 912539-16-3 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[2-(3-pyrrolidinyl)oxy]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)



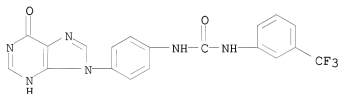
RN 912539-17-4 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[3-(trifluoromethyl)phenyl]-  
(CA INDEX NAME)



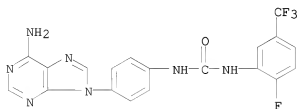
RN 912539-18-5 CAPLUS

CN Urea, N-[4-(1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]-N'-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



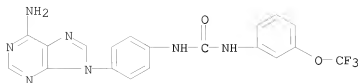
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CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[2-fluoro-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)



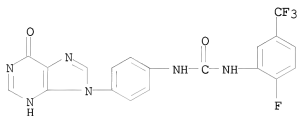
RN 912539-20-9 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[3-(trifluoromethoxy)phenyl]-  
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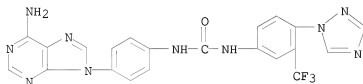
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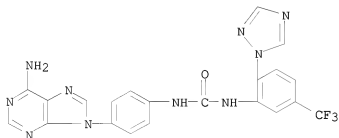
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CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-(4-(1H-1,2,4-triazol-1-yl)-3-(trifluoromethyl)phenyl)- (CA INDEX NAME)



RN 912539-24-3 CAPLUS

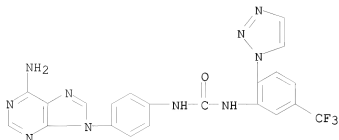
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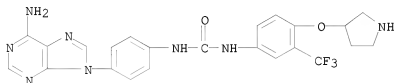
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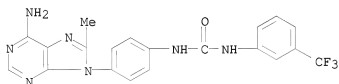
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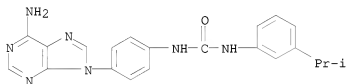
RN 912539-27-6 CAPLUS

CN Urea, N-[4-(6-amino-8-methyl-9H-purin-9-yl)phenyl]-N'-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 912539-29-8 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[3-(1-methylethyl)phenyl]- (CA INDEX NAME)



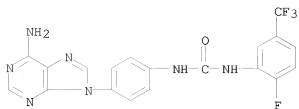
RN 912539-40-3 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[2-fluoro-5-(trifluoromethyl)phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

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CRN 912539-19-6

CMF C19 H13 F4 N7 O



CM 2

CRN 76-05-1

CMF C2 H F3 O2



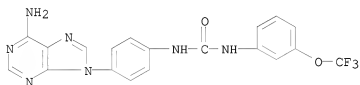
RN 912539-41-4 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[3-(trifluoromethoxy)phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

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CRN 912539-20-9

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CM 2

CRN 76-05-1

CMF C2 H F3 O2

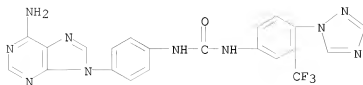


RN 912539-43-6 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[4-(1H-1,2,4-triazol-1-yl)-3-(trifluoromethyl)phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

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CRN 912539-23-2  
CMF C21 H15 F3 N10 O

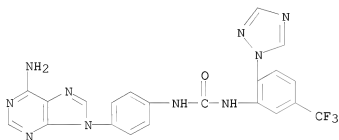


CM 2  
CRN 76-05-1  
CMF C2 H F3 O2



RN 912539-44-7 CAPLUS  
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CRN 912539-24-3  
CMF C21 H15 F3 N10 O



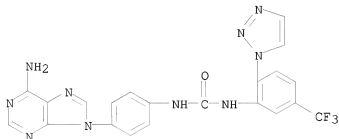
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CRN 76-05-1  
CMF C2 H F3 O2



RN 912539-45-8 CAPLUS  
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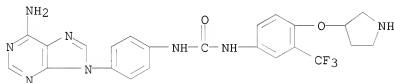


CM 2

CRN 76-05-1  
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RN 912539-46-9 CAPLUS  
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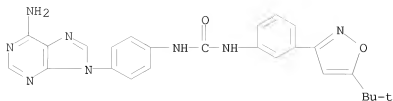


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RN 912539-48-1 CAPLUS  
 CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[3-[5-(1,1-dimethylethyl)-3-isoxazolyl]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

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CM 2

CRN 76-05-1

CMF C2 H F3 O2

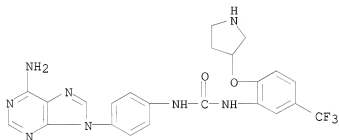


IT 912539-36-7P 912539-37-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of purine derivs. as receptor-tyrosine kinase activity  
inhibitors)

RN 912539-36-7 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[2-(3-pyrrolidinyloxy)-5-(trifluoromethyl)phenyl]-, hydrochloride (1:2) (CA INDEX NAME)



● 2 HCl

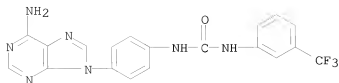
RN 912539-37-8 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[3-(trifluoromethyl)phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 912539-17-4

CMF C19 H14 F3 N7 O



CM 2

CRN 76-05-1  
CMF C2 H F3 O2



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2009 ACS on SIN

ACCESSION NUMBER: 2005:962206 CAPLUS

DOCUMENT NUMBER: 143:266944

TITLE: Preparation of heteroarylphenylurea derivatives as Raf inhibitors

INVENTOR(S): Oikawa, Nobuhiro; Mizuguchi, Eisaku; Morikami, Kenji; Shimma, Nobuo; Ishii, Nobuya; Tsukaguchi, Toshiyuki; Ozawa, Sawako

PATENT ASSIGNEE(S): Chugai Seiyaku Kabushiki Kaisha, Japan

SOURCE: PCI Int. Appl., 296 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005080330	A1	20050901	WO 2005-JP2923	20050223
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
EP 1724258	A1	20061122	EP 2005-719431	20050223
R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR			
US 20080119466	A1	20080522	US 2006-590026	20060818
PRIORITY APPLN. INFO.:			JP 2004-47037	A 20040223
			JP 2004-248856	A 20040827

OTHER SOURCE(S):

MARPAT 143:266944

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

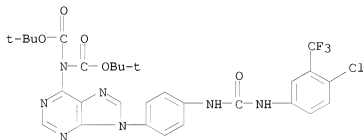
AB Title compds. I [R1, R2, R5 = H, halo, etc.; R3, R4 = H, halo, etc.; R6, R7 = H, halo; Z1, Z2 = H, OH, etc.; Q = II; G1 = C-Y2, N; ring A = benzene, etc.; Y1, Y2 = H, halo, etc.] were prepared For example, treatment of 1-[4-(6-aminopurin-9-yl)phenyl]-3-[4-chloro-3-(trifluoromethyl)phenyl]urea hydrochloride, e.g., prepared from adenine in 5 steps, with propylisocyanate afforded compound III. In Raf-1 enzyme inhibition assays, the IC50 value of compound III was 0.013  $\mu$ M. Cpmpounds I are claimed useful for the treatment of cancer, diabetes, etc.

IT 863673-35-2P 863673-36-3P 863673-42-1P  
 863673-54-5P 863673-58-9P 863673-68-1P  
 863674-28-6P 863674-35-5P 863674-36-6P  
 863674-48-0P 863674-50-4P 863674-56-0P  
 863674-57-1P 863674-58-2P 863675-11-0P  
 863675-12-1P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (preparation of heteroarylphenylurea derivs. as Raf inhibitors for treatment of cancer and diabetes)

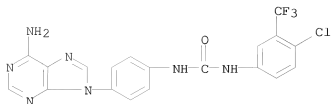
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CN Imidodicarbonic acid, 2-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, 1,3-bis(1,1-dimethylethyl) ester (CA INDEX NAME)



RN 863673-36-3 CAPLUS

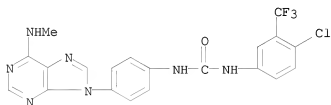
CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 863673-42-1 CAPLUS

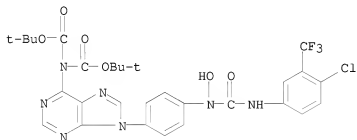
CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 863673-54-5 CAPLUS

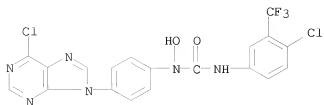
CN Imidodicarbonic acid, 2-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]hydroxyamino]phenyl]-9H-purin-6-yl]-, 1,3-bis(1,1-dimethylethyl) ester (CA INDEX NAME)



RN 863673-58-9 CAPLUS

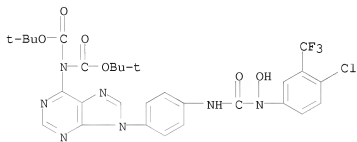
CN Urea, N-[4-(6-chloro-9H-purin-9-yl)phenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]-N-hydroxy- (CA INDEX NAME)





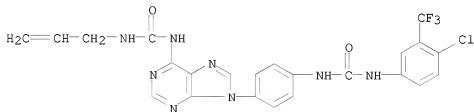
RN 863673-68-1 CAPLUS

CN Imidodicarbonic acid, 2-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]hydroxyamino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, 1,3-bis(1,1-dimethylethyl) ester (CA INDEX NAME)



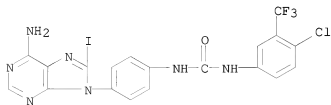
RN 863674-28-6 CAPLUS

CN Urea, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-N'-2-propen-1-yl- (CA INDEX NAME)



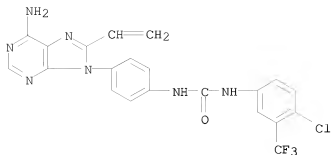
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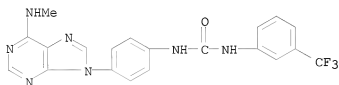
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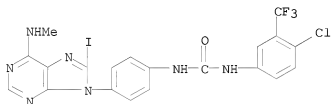
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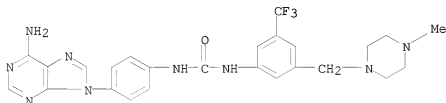
RN 863674-50-4 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[8-iodo-6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



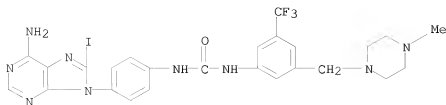
RN 863674-56-0 CAPLUS

CN Urea, N-[4-(6-amino-8-iodo-9H-purin-9-yl)phenyl]-N'-[3-[(4-methyl-1-piperazinyl)methyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)



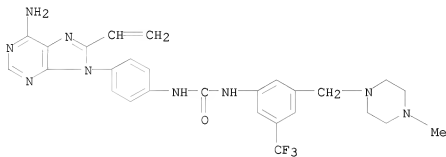
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CN Urea, N-[4-(6-amino-8-iodo-9H-purin-9-yl)phenyl]-N'-[3-[(4-methyl-1-piperazinyl)methyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)



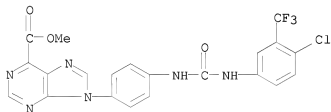
RN 863674-58-2 CAPLUS

CN Urea, N-[4-(6-amino-8-ethenyl-9H-purin-9-yl)phenyl]-N'-[3-[(4-methyl-1-piperazinyl)methyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)



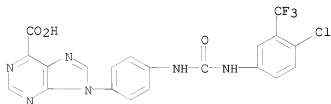
RN 863675-11-0 CAPLUS

CN 9H-Purine-6-carboxylic acid, 9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-, methyl ester (CA INDEX NAME)



RN 863675-12-1 CAPLUS

CN 9H-Purine-6-carboxylic acid, 9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]- (CA INDEX NAME)



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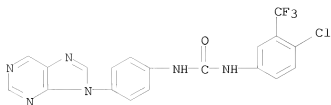
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of heteroarylphenylurea derivs. as Raf inhibitors for treatment of cancer and diabetes)

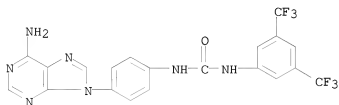
RN 863673-11-4 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-(9H-purin-9-yl)phenyl]-  
(CA INDEX NAME)



RN 863673-37-4 CAPLUS

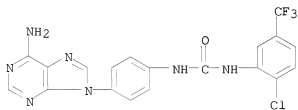
CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[3,5-bis(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 863673-38-5 CAPLUS

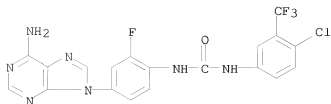
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● HCl

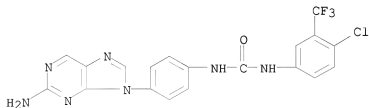
RN 863673-39-6 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)-2-fluorophenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



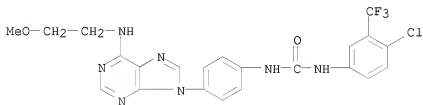
● HCl

RN 863673-40-9 CAPLUS  
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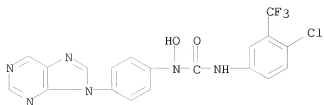
● HCl

RN 863673-41-0 CAPLUS  
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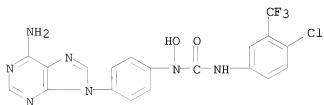


● HCl

RN 863673-53-4 CAPLUS  
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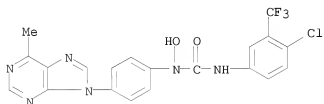


RN 863673-55-6 CAPLUS  
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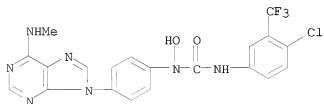


● HCl

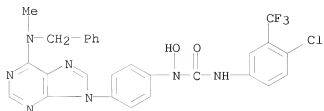
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RN 863673-59-0 CAPLUS  
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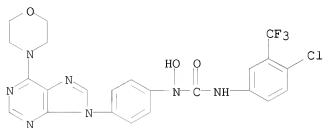


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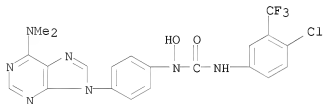
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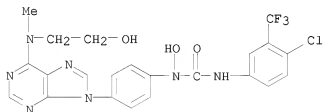
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RN 863673-63-6 CAPLUS

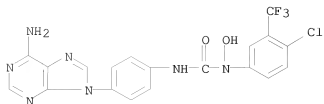
CN Urea, N'-(4-chloro-3-(trifluoromethyl)phenyl)-N-hydroxy-N-[4-[6-[(2-hydroxyethyl)methylamino]-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



RN 863673-69-2 CAPLUS

CN Urea, N'-(4-(6-amino-9H-purin-9-yl)phenyl)-N-[4-chloro-3-(trifluoromethyl)phenyl]-N-hydroxy-, hydrochloride (1:1) (CA INDEX NAME)

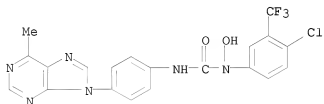




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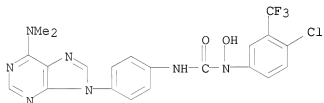
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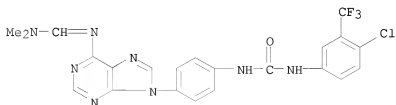
RN 863673-74-9 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[6-(dimethylamino)-9H-purin-9-yl]phenyl]-N-hydroxy- (CA INDEX NAME)



RN 863674-01-5 CAPLUS

CN Methanimidamide, N'-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-N,N-dimethyl-, hydrochloride (1:1) (CA INDEX NAME)

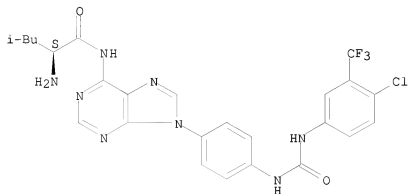


● HCl

RN 863674-02-6 CAPLUS

CN Pentanamide, 2-amino-N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-4-methyl-, hydrochloride (1:1), (2S)- (CA INDEX NAME)

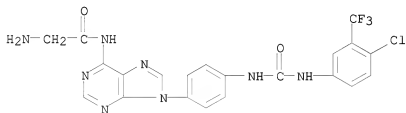
Absolute stereochemistry.



● HCl

RN 863674-03-7 CAPLUS

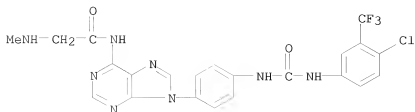
CN Acetamide, 2-amino-N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 863674-04-8 CAPLUS

CN Acetamide, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-2-(methylamino)-, hydrochloride (1:1) (CA INDEX NAME)

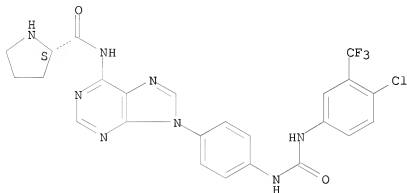


● HCl

RN 863674-05-9 CAPLUS

CN 2-Pyrrolidinecarboxamide, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, hydrochloride (1:1), (2S)- (CA INDEX NAME)

Absolute stereochemistry.

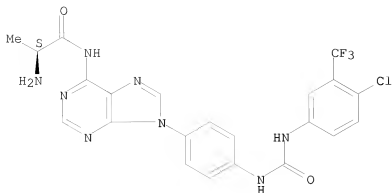


● HCl

RN 863674-06-0 CAPLUS

CN Propanamide, 2-amino-N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, hydrochloride (1:1), (2S)- (CA INDEX NAME)

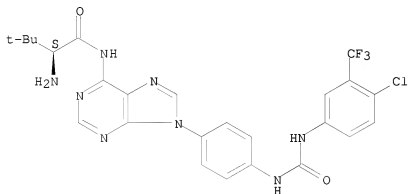
Absolute stereochemistry.



● HCl

RN 863674-07-1 CAPLUS  
 CN Butanamide, 2-amino-N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-3,3-dimethyl-, hydrochloride (1:1), (2S)- (CA INDEX NAME)

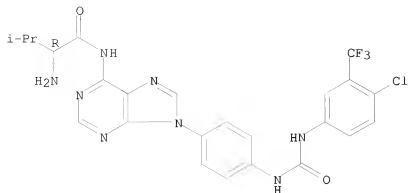
Absolute stereochemistry.



● HCl

RN 863674-08-2 CAPLUS  
 CN Butanamide, 2-amino-N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-3-methyl-, hydrochloride (1:1), (2R)- (CA INDEX NAME)

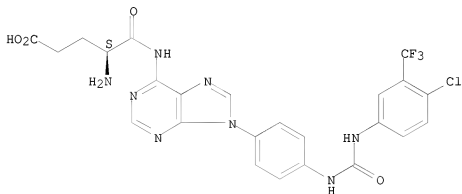
Absolute stereochemistry.



● HCl

RN 863674-09-3 CAPLUS  
 CN Pentanoic acid, 4-amino-5-[[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]amino]-5-oxo-, hydrochloride (1:1), (4S)- (CA INDEX NAME)

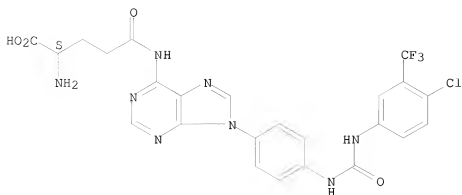
Absolute stereochemistry.



● HCl

RN 863674-10-6 CAPLUS  
 CN L-Glutamine, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, monohydrochloride (9CI) (CA INDEX NAME)

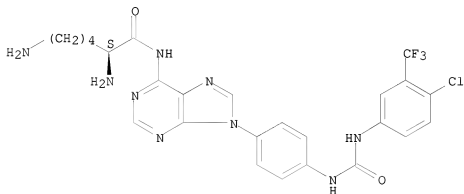
Absolute stereochemistry.



● HCl

RN 863674-11-7 CAPLUS  
 CN Hexanamide, 2,6-diamino-N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, hydrochloride (1:2), (2S)- (CA INDEX NAME)

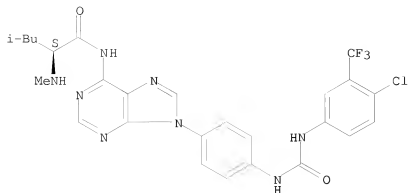
Absolute stereochemistry.



● 2 HCl

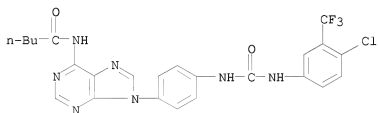
RN 863674-12-8 CAPLUS  
 CN Pentanamide, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-4-methyl-2-(methylamino)-, hydrochloride (1:1), (2S)- (CA INDEX NAME)

Absolute stereochemistry.

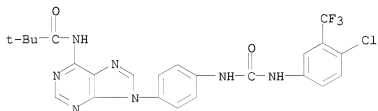


● HCl

RN 863674-13-9 CAPLUS  
 CN Pentanamide, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]- (CA INDEX NAME)



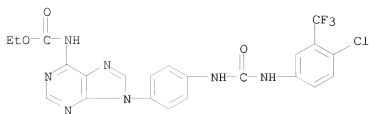
RN 863674-14-0 CAPLUS  
 CN Propanamide, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-2,2-dimethyl- (CA INDEX NAME)



RN 863674-15-1 CAPLUS  
 CN Acetamide, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-2-[2-(2-methoxyethoxy)ethoxy]- (CA INDEX NAME)

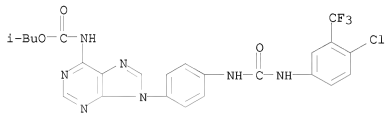






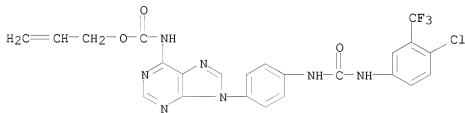
RN 863674-19-5 CAPLUS

CN Carbamic acid, [9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, 2-methylpropyl ester (9CI) (CA INDEX NAME)



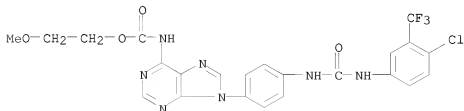
RN 863674-20-8 CAPLUS

CN Carbamic acid, [9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, 2-propenyl ester (9CI) (CA INDEX NAME)



RN 863674-21-9 CAPLUS

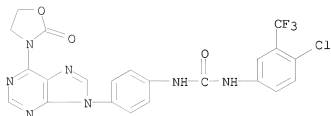
CN Carbamic acid, [9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, 2-methoxyethyl ester (9CI) (CA INDEX NAME)



RN 863674-22-0 CAPLUS

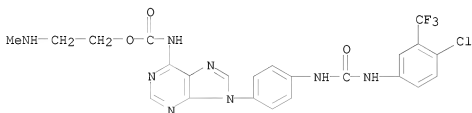
CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[6-(2-oxo-3-

oxazolidinyl)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



RN 863674-23-1 CAPLUS

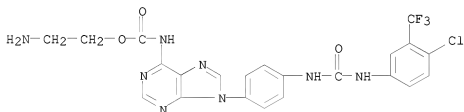
CN Carbamic acid, [9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, 2-(methylamino)ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 863674-24-2 CAPLUS

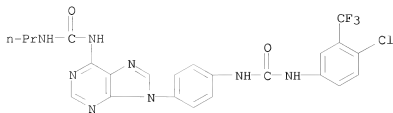
CN Carbamic acid, [9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, 2-aminoethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

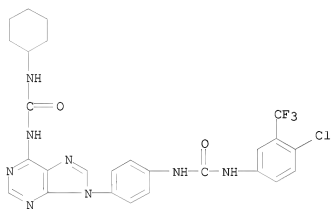
RN 863674-25-3 CAPLUS

CN Urea, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-N'-propyl- (CA INDEX NAME)



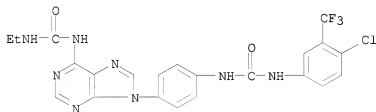
RN 863674-26-4 CAPLUS

CN Urea, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-N'-cyclohexyl- (CA INDEX NAME)



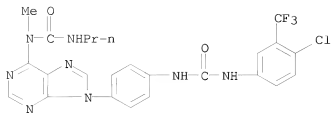
RN 863674-27-5 CAPLUS

CN Urea, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-N'-ethyl- (CA INDEX NAME)



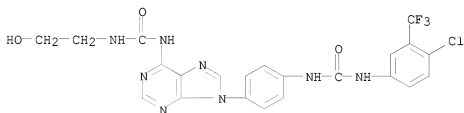
RN 863674-29-7 CAPLUS

CN Urea, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-N-methyl-N'-propyl- (CA INDEX NAME)



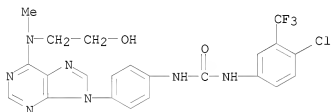
RN 863674-30-0 CAPLUS

CN Urea, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-N'-(2-hydroxyethyl)- (CA INDEX NAME)



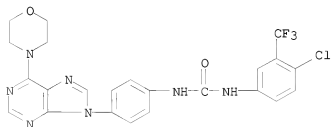
RN 863674-31-1 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[6-[(2-hydroxyethyl)methylamino]-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



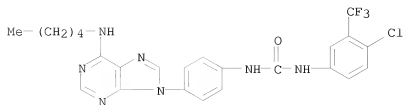
RN 863674-32-2 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[6-(4-morpholinyl)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



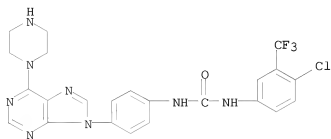
RN 863674-33-3 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[6-(pentylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



RN 863674-34-4 CAPLUS

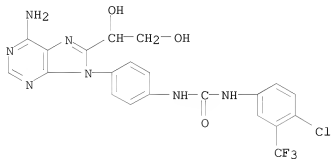
CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-{6-(1-piperazinyl)-9H-purin-9-yl}phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

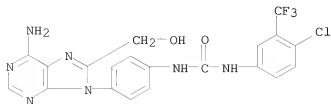
RN 863674-37-7 CAPLUS

CN Urea, N-[4-{6-amino-8-(1,2-dihydroxyethyl)-9H-purin-9-yl}phenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



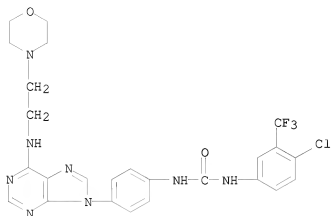
RN 863674-38-8 CAPLUS

CN Urea, N-[4-{6-amino-8-(hydroxymethyl)-9H-purin-9-yl}phenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



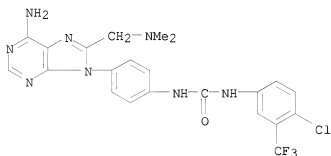
RN 863674-39-9 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[6-[[2-(4-morpholinyl)ethyl]amino]-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



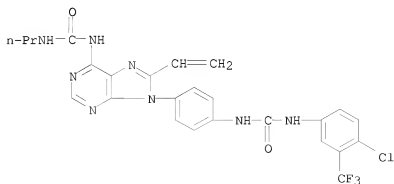
RN 863674-40-2 CAPLUS

CN Urea, N-[4-[6-amino-8-[(dimethylamino)methyl]-9H-purin-9-yl]phenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



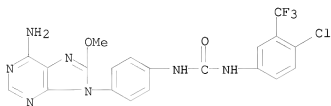
RN 863674-41-3 CAPLUS

CN Urea, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-8-ethenyl-9H-purin-6-yl]-N'-propyl- (CA INDEX NAME)



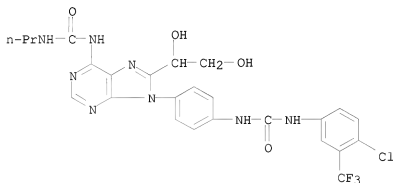
RN 863674-42-4 CAPLUS

CN Urea, N-[4-(6-amino-8-methoxy-9H-purin-9-yl)phenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



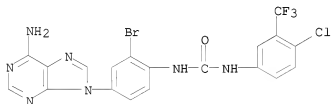
RN 863674-43-5 CAPLUS

CN Urea, N-[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-8-(1,2-dihydroxyethyl)-9H-purin-6-yl]-N'-propyl- (CA INDEX NAME)



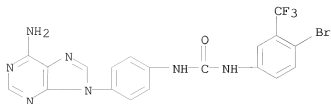
RN 863674-44-6 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)-2-bromophenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 863674-45-7 CAPLUS

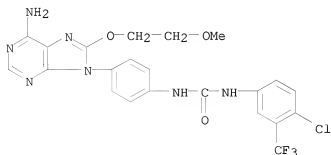
CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[4-bromo-3-(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

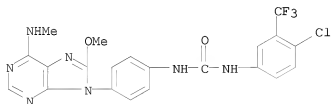
RN 863674-46-8 CAPLUS

CN Urea, N-[4-{6-amino-8-(2-methoxyethoxy)-9H-purin-9-yl}phenyl]-N'-(4-chloro-3-(trifluoromethyl)phenyl)- (CA INDEX NAME)



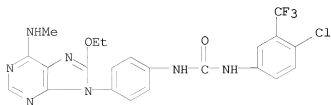
RN 863674-51-5 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-(4-{8-methoxy-6-(methylamino)-9H-purin-9-yl}phenyl)- (CA INDEX NAME)



RN 863674-52-6 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-(4-{8-ethoxy-6-(methylamino)-9H-purin-9-yl}phenyl)- (CA INDEX NAME)

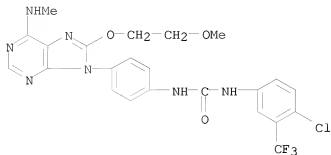


RN 863674-53-7 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-(4-{8-(2-methoxyethoxy)-6-(methylamino)-9H-purin-9-yl}phenyl)- (CA INDEX NAME)

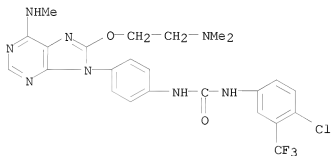


(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



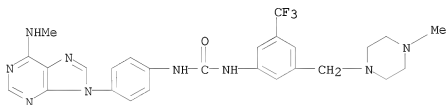
RN 863674-54-8 CAPLUS

CN Urea, N-[4-chloro-3-(trifluoromethyl)phenyl]-N'-[4-[8-[2-(dimethylamino)ethoxy]-6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



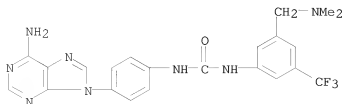
RN 863674-55-9 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[3-[(4-methyl-1-piperazinyl)methyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)



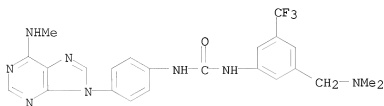
RN 863674-59-3 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[3-[(dimethylamino)methyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)



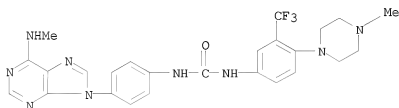
RN 863674-60-6 CAPLUS

CN Urea, N-[3-[(dimethylamino)methyl]-5-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



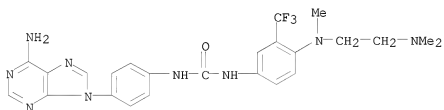
RN 863674-65-1 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-(4-methyl-1-piperazinyl)-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



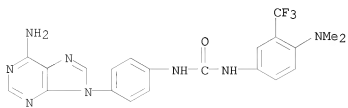
RN 863674-66-2 CAPLUS

CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[4-[[2-(dimethylamino)ethyl]methylamino]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 863674-67-3 CAPLUS

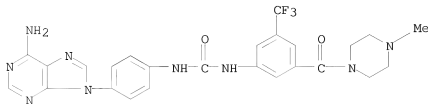
CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[4-(dimethylamino)-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 863674-68-4 CAPLUS

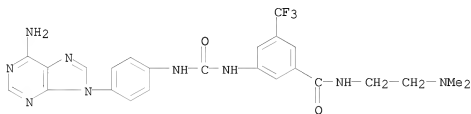
CN Urea, N-[4-(6-amino-9H-purin-9-yl)phenyl]-N'-[3-[4-methyl-1-

piperazinyl)carbonyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)



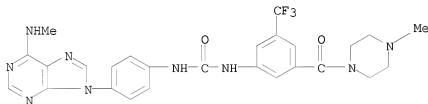
RN 863674-69-5 CAPLUS

CN Benzamide, 3-[[[4-(6-amino-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-N-[2-(dimethylamino)ethyl]-5-(trifluoromethyl)- (CA INDEX NAME)



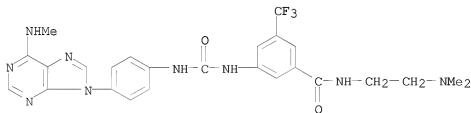
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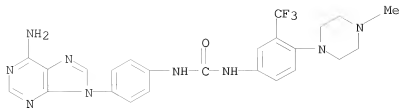
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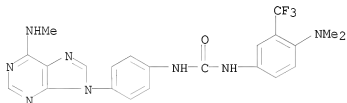
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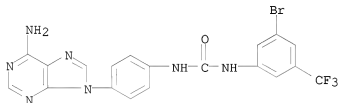
RN 863674-73-1 CAPLUS

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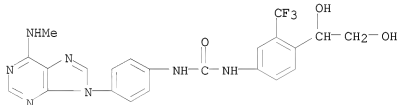
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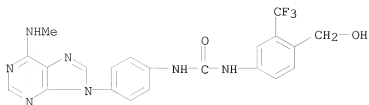
RN 863674-75-3 CAPLUS

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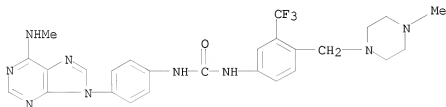
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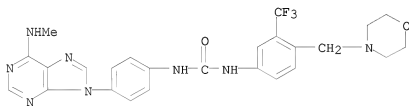
RN 863674-77-5 CAPLUS

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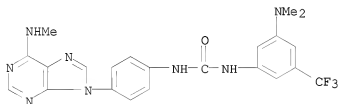
RN 863674-78-6 CAPLUS

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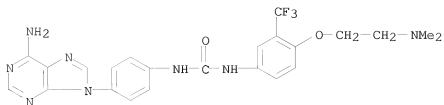
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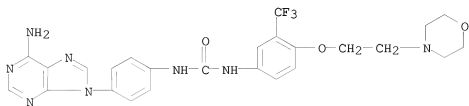
RN 863674-80-0 CAPLUS

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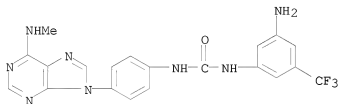
RN 863674-81-1 CAPLUS

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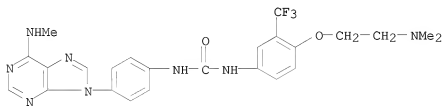
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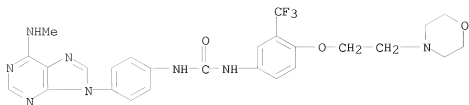
RN 863674-83-3 CAPLUS

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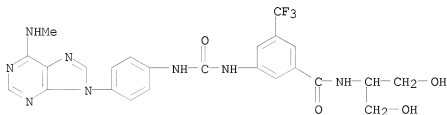
RN 863674-84-4 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[2-(4-morpholinyl)ethoxy]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



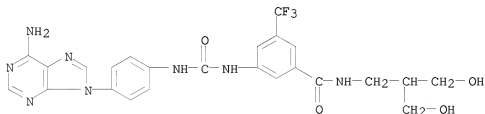
RN 863674-85-5 CAPLUS

CN Benzamide, N-[2-hydroxy-1-(hydroxymethyl)ethyl]-3-[[[4-[6-(methylamino)-9H-purin-9-yl]phenyl]amino]carbonyl]amino]-5-(trifluoromethyl)- (CA INDEX NAME)



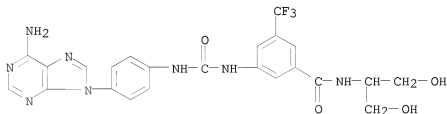
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CN Benzamide, 3-[[[4-(6-amino-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-N-[3-hydroxy-2-(hydroxymethyl)propyl]-5-(trifluoromethyl)- (CA INDEX NAME)



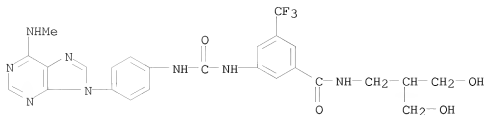
RN 863674-87-7 CAPLUS

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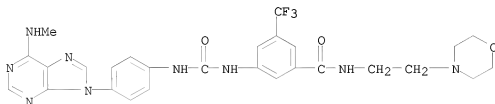
RN 863674-88-8 CAPLUS

CN Benzamide, N-[3-hydroxy-2-(hydroxymethyl)propyl]-3-[[[4-[6-(methylamino)-9H-purin-9-yl]phenyl]amino]carbonyl]amino]-5-(trifluoromethyl)- (CA INDEX NAME)



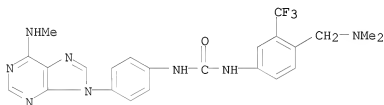
RN 863674-89-9 CAPLUS

CN Benzamide, 3-[[[4-[6-(methylamino)-9H-purin-9-yl]phenyl]amino]carbonyl]amino]-N-[2-(4-morpholinyl)ethyl]-5-(trifluoromethyl)- (CA INDEX NAME)



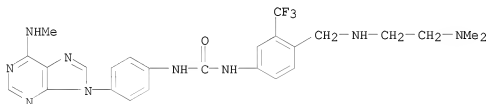
RN 863674-90-2 CAPLUS

CN Urea, N-[4-[(dimethylamino)methyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



RN 863674-91-3 CAPLUS

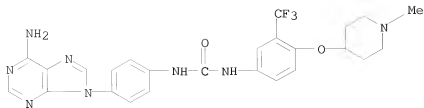
CN Urea, N-[4-[[2-(dimethylamino)ethyl]amino]methyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



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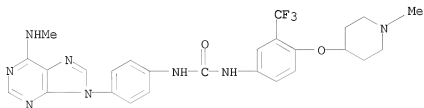
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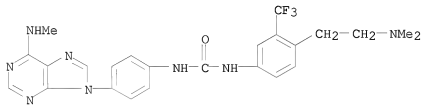
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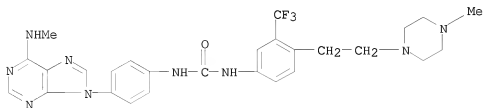
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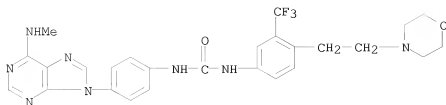
RN 863674-95-7 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[2-(4-methyl-1-piperazinyl)ethyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



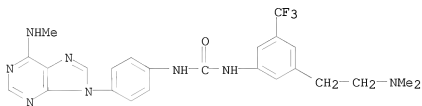
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CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[2-(4-morpholinyl)ethyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



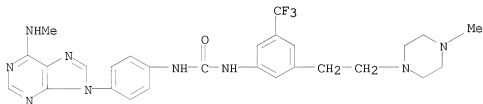
RN 863674-97-9 CAPLUS

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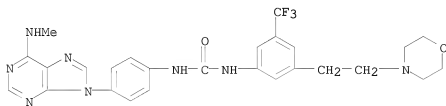
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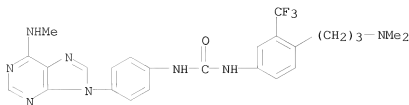
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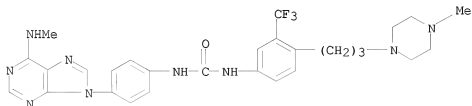
RN 863675-00-7 CAPLUS

CN Urea, N-[4-[3-(dimethylamino)propyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



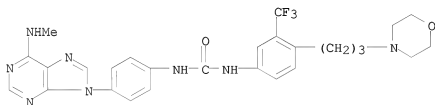
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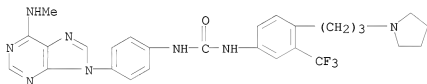
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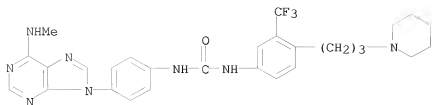
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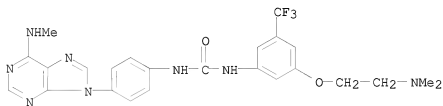
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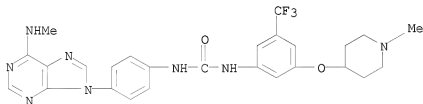
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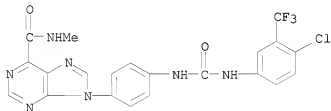
RN 863675-06-3 CAPLUS

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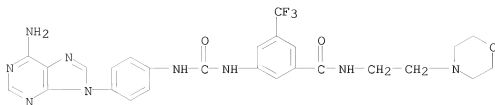
RN 863675-13-2 CAPLUS

CN 9H-Purine-6-carboxamide, 9-[4-[[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-N-methyl- (CA INDEX NAME)



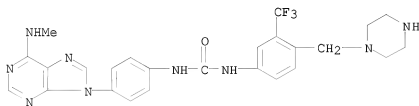
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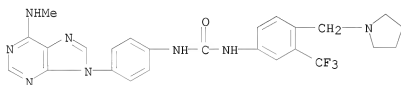
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CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-(1-piperazinylmethyl)-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



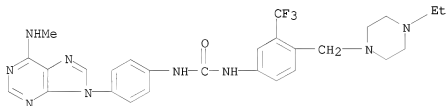
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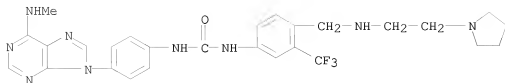
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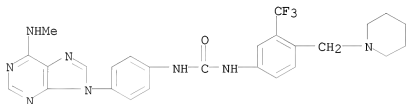
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CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[[[2-(1-pyrrolidinyl)ethyl]amino]methyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



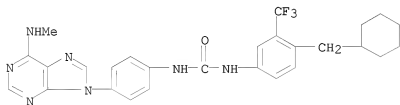
RN 863675-22-3 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-(1-piperidinylmethyl)-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



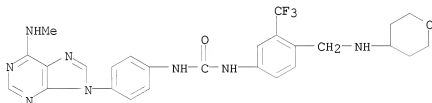
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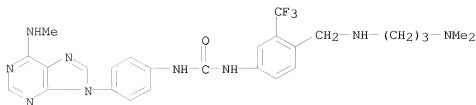
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CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[(1-tetrahydro-2H-pyran-4-yl)amino]methyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



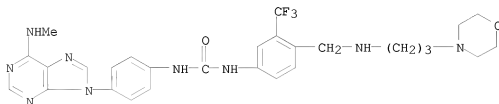
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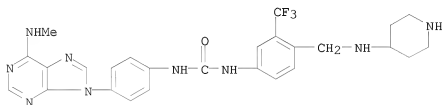
RN 863675-27-8 CAPLUS

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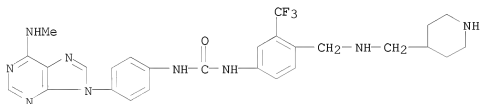
RN 863675-28-9 CAPLUS

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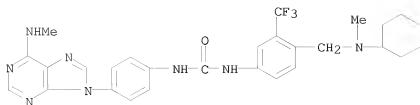
RN 863675-29-0 CAPLUS

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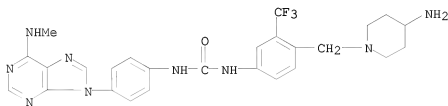
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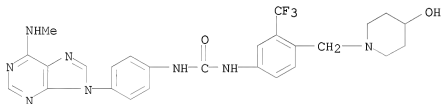
RN 863675-31-4 CAPLUS

CN Urea, N-[4-[(4-amino-1-piperidinyl)methyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



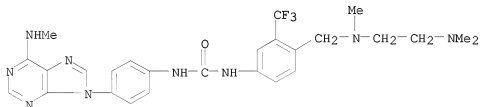
RN 863675-32-5 CAPLUS

CN Urea, N-[4-[(4-hydroxy-1-piperidinyl)methyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



RN 863675-33-6 CAPLUS

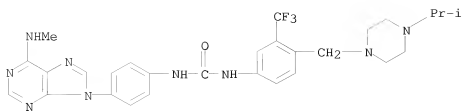
CN Urea, N-[4-[[2-(dimethylamino)ethyl]methylamino]methyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



RN 863675-34-7 CAPLUS

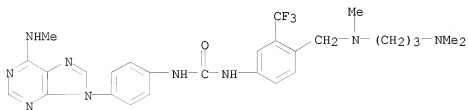
CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[[4-(1-methylethyl)-1-piperazinyl]methyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)





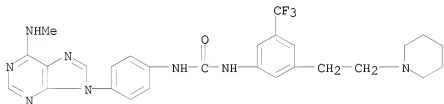
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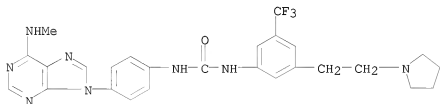
RN 863675-36-9 CAPLUS

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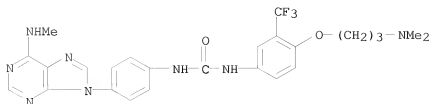
RN 863675-37-0 CAPLUS

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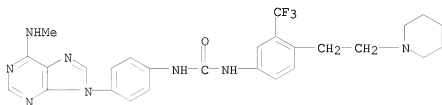
RN 863675-38-1 CAPLUS

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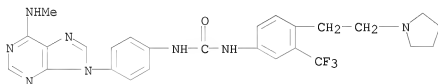
RN 863675-39-2 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[2-(1-piperidinyl)ethyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



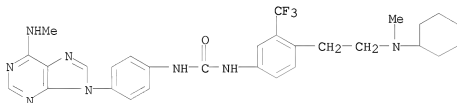
RN 863675-40-5 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[2-(1-pyrrolidinyl)ethyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



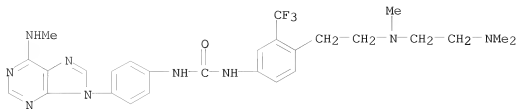
RN 863675-41-6 CAPLUS

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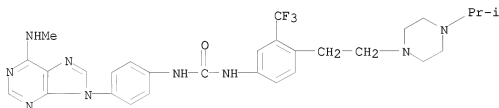
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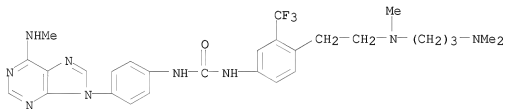
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CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[2-[4-(1-methylethyl)-1-piperazinyl]ethyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



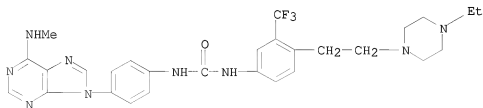
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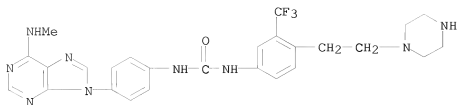
RN 863675-45-0 CAPLUS

CN Urea, N-[4-[2-(4-ethyl-1-piperazinyl)ethyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



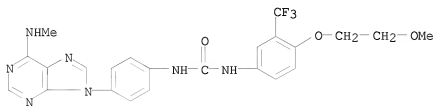
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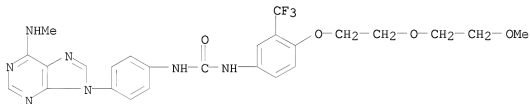
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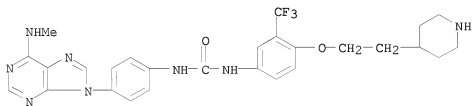
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CN Urea, N-[4-(2-(2-methoxyethoxy)ethoxy)-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



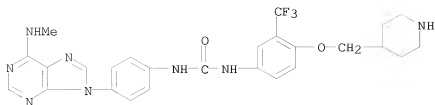
RN 863675-49-4 CAPLUS

CN Urea, N-[4-[2-(4-piperidinyloxy)ethoxy]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



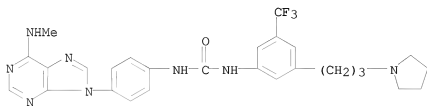
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CN Urea, N-[4-(4-piperidinylmethoxy)-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



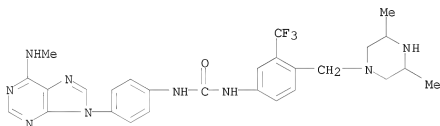
RN 863675-51-8 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[3-[3-(1-pyrrolidinyl)propyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)



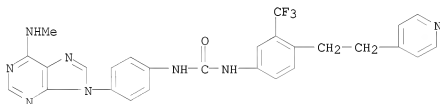
RN 863675-52-9 CAPLUS

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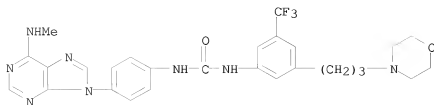
RN 863675-53-0 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[2-(4-pyridinyl)ethyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



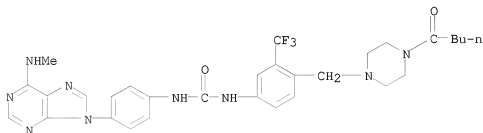
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CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[3-[3-(4-morpholinyl)propyl]-5-(trifluoromethyl)phenyl]- (CA INDEX NAME)



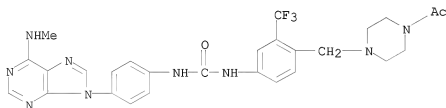
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CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-[(1-oxopentyl)-1-piperazinyl]methyl]-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



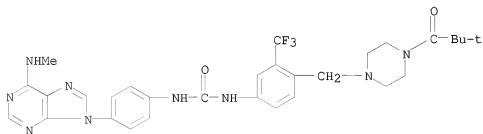
RN 863675-56-3 CAPLUS

CN Urea, N-[4-[(4-acetyl-1-piperazinyl)methyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



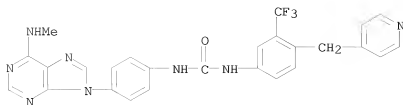
RN 863675-57-4 CAPLUS

CN Urea, N-[4-[(4-(2,2-dimethyl-1-oxopropyl)-1-piperazinyl)methyl]-3-(trifluoromethyl)phenyl]-N'-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]- (CA INDEX NAME)



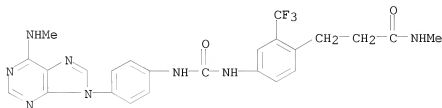
RN 863675-58-5 CAPLUS

CN Urea, N-[4-[6-(methylamino)-9H-purin-9-yl]phenyl]-N'-[4-(4-pyridinylmethyl)-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 863675-59-6 CAPLUS

CN Benzenepropanamide, N-methyl-4-[[[4-[6-(methylamino)-9H-purin-9-yl]phenyl]amino]carbonyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)



IT 863675-80-3P

863675-81-4P

863675-82-5P

863675-83-6P

863675-90-5P

863675-93-8P

863675-94-9P

863675-95-0P

863675-96-1P

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863676-03-3P

863676-06-6P

863676-07-7P

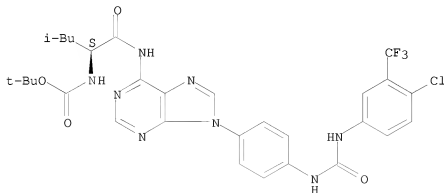
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of heteroarylphenylurea derivs. as Raf inhibitors for treatment of cancer and diabetes)

RN 863675-80-3 CAPLUS

CN Carbamic acid, [(1S)-1-[[[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]amino]carbonyl]-3-methylbutyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

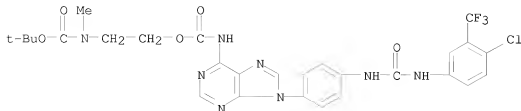
Absolute stereochemistry.



RN 863675-81-4 CAPLUS

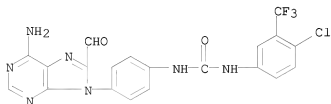
CN Carbamic acid, [2-[[[9-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]amino]carbonyl]oxy]ethyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA

INDEX NAME)



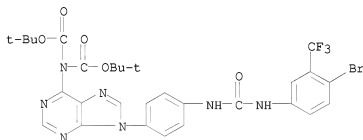
RN 863675-82-5 CAPLUS

CN Urea, N-[4-(6-amino-8-formyl-9H-purin-9-yl)phenyl]-N'-[4-chloro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



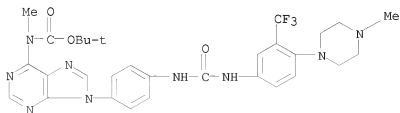
RN 863675-83-6 CAPLUS

CN Imidodicarbonic acid, 2-[9-[4-[[[4-bromo-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, 1,3-bis(1,1-dimethylethyl) ester (CA INDEX NAME)



RN 863675-90-5 CAPLUS

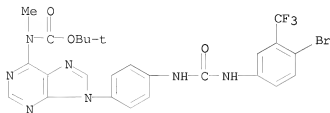
CN Carbamic acid, methyl[9-[4-[[[4-(4-methyl-1-piperazinyl)-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 863675-93-8 CAPLUS

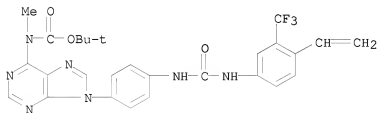


CN Carbamic acid, [9-[4-[[[4-bromo-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl)methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



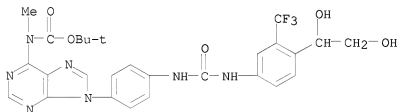
RN 863675-94-9 CAPLUS

CN Carbamic acid, [9-[4-[[[4-ethenyl-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl)methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



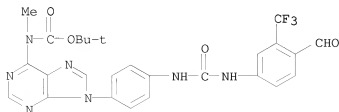
RN 863675-95-0 CAPLUS

CN Carbamic acid, [9-[4-[[[4-(1,2-dihydroxyethyl)-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl)methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



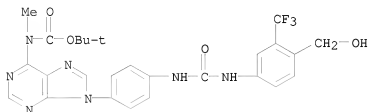
RN 863675-96-1 CAPLUS

CN Carbamic acid, [9-[4-[[[4-formyl-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl)methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



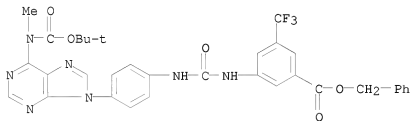
RN 863675-97-2 CAPLUS

CN Carbamic acid, [9-[4-[[[4-(hydroxymethyl)-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl)methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



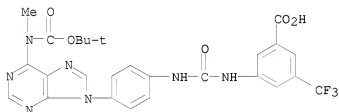
RN 863676-01-1 CAPLUS

CN Benzoic acid, 3-[[[4-[6-[[[(1,1-dimethylethoxy)carbonyl]methylamino]-9H-purin-9-yl]phenyl]amino]carbonyl]amino]-5-(trifluoromethyl)-, phenylmethyl ester (CA INDEX NAME)



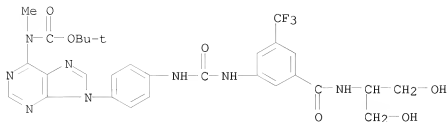
RN 863676-02-2 CAPLUS

CN Benzoic acid, 3-[[[4-[6-[[[(1,1-dimethylethoxy)carbonyl]methylamino]-9H-purin-9-yl]phenyl]amino]carbonyl]amino]-5-(trifluoromethyl)- (CA INDEX NAME)



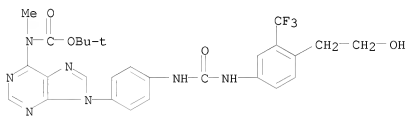
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CN Carbamic acid, [9-[4-[[[3-[[[2-hydroxy-1-(hydroxymethyl)ethyl]amino]carbonyl]-5-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl)methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



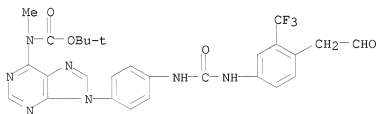
RN 863676-06-6 CAPLUS

CN Carbamic acid, [9-[4-[[[4-(2-hydroxyethyl)-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 863676-07-7 CAPLUS

CN Carbamic acid, methyl[9-[4-[[[4-(2-oxoethyl)-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenyl]-9H-purin-6-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2003:319714 CAPLUS

DOCUMENT NUMBER: 138:338157

TITLE: Preparation of 1,4-disubstituted benzo-fused ureas as cytokine inhibitors

INVENTOR(S): Cirillo, Pier F.; Hammach, Abdelhakim; Regan, John R.

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 100 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003032989	A1	20030424	WO 2002-US32809	20021011
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG			
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AU 2002335012	A1	20030428	AU 2002-335012	20021011
US 20030162968	A1	20030828	US 2002-269173	20021011
US 6825184	B2	20041130		
EP 1438048	A1	20040721	EP 2002-801703	20021011
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JP 2005506350	T	20050303	JP 2003-535792	20021011
PRIORITY APPLN. INFO.:			US 2001-330254P	P 20011018
			WO 2002-US32809	W 20021011
OTHER SOURCE(S):		MARPAT 138:338157		
GI				

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The title compds. [I; ring A = fused (un)saturated ring containing 3-5 carbon atoms (wherein ring A or the Ph ring to which it is fused is optionally substituted); G = (un)substituted 5-membered heteroaryl; Q = (un)substituted naphthyl, benzocyclobutanyl, indanyl, etc.; X = O, S] which are active as anti-inflammatory agents, were prepared. Thus, reacting the carbamate II with the amine III (multi-step preparation given) in DMSO afforded 84% urea IV. The preferred compds. I including those from the synthetic examples were evaluated for their inhibition of TNF $\alpha$  production in THP cells, and showed IC50 < 10  $\mu$ M.

IT

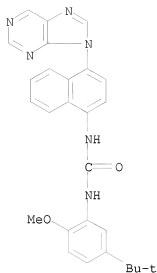
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515843-87-5P	515843-88-6P	515843-89-7P
515843-90-0P	515843-91-1P	515843-92-2P
515843-93-3P	515843-94-4P	515843-95-5P
515843-96-6P	515843-97-7P	515843-98-8P
515843-99-9P	515844-00-5P	515844-01-6P
515844-02-7P	515844-04-9P	

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 1,4-disubstituted benzo-fused ureas as cytokine inhibitors)

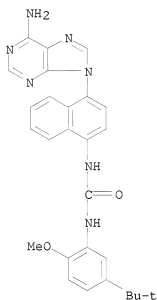
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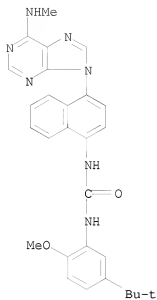
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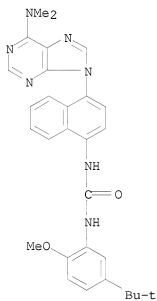
RN 515843-80-8 CAPLUS

CN Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-(4-[6-(methylamino)-9H-purin-9-yl]-1-naphthalenyl)- (CA INDEX NAME)



RN 515843-81-9 CAPLUS

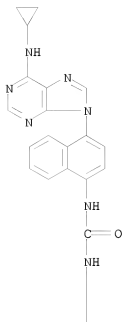
CN Urea, N-[4-[6-(dimethylamino)-9H-purin-9-yl]-1-naphthalenyl]-N'-[5-(1,1-dimethylethyl)-2-methoxyphenyl]- (CA INDEX NAME)



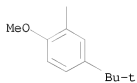
RN 515843-82-0 CAPLUS

CN Urea, N-[4-[6-(cyclopropylamino)-9H-purin-9-yl]-1-naphthalenyl]-N'-[5-(1,1-dimethylethyl)-2-methoxyphenyl]- (CA INDEX NAME)

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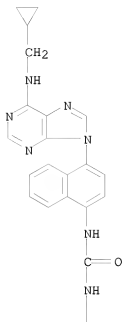


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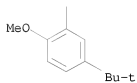


RN 515843-83-1 CAPLUS  
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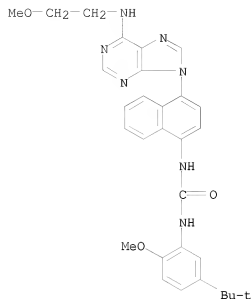


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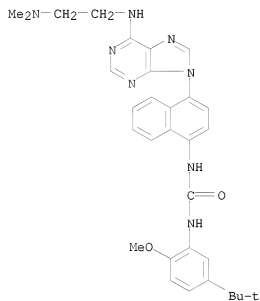


RN 515843-84-2 CAPLUS  
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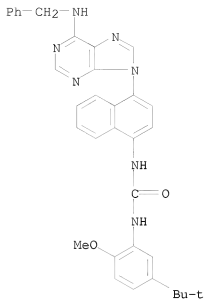




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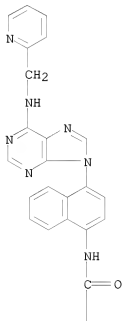
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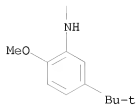
RN 515843-87-5 CAPLUS

CN Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-{6-[(2-pyridinylmethyl)amino]-9H-purin-9-yl]-1-naphthalenyl]- (CA INDEX NAME)

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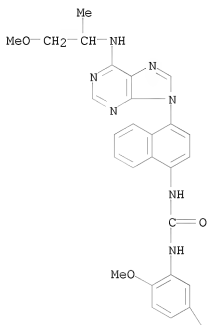


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RN 515843-88-6 CAPLUS  
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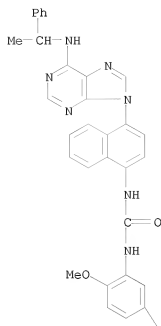
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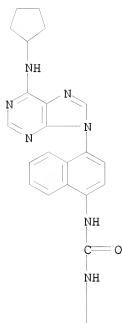
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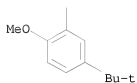
Bu-t

RN 515843-90-0 CAPLUS  
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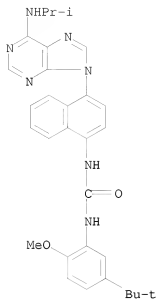
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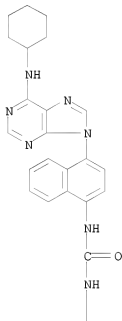
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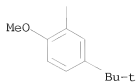
RN 515843-92-2 CAPLUS

CN Urea, N-[4-[6-(cyclohexylamino)-9H-purin-9-yl]-1-naphthalenyl]-N'-[5-(1,1-dimethylethyl)-2-methoxyphenyl]- (CA INDEX NAME)

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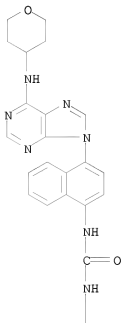
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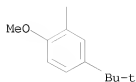
RN 515843-93-3 CAPLUS

CN Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-[6-[(tetrahydro-2H-pyran-4-yl)amino]-9H-purin-9-yl]-1-naphthalenyl]- (CA INDEX NAME)

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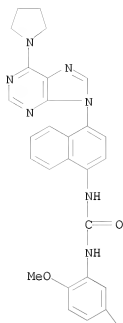
RN 515843-94-4 CAPLUS

CN Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-[6-[(tetrahydro-3-furanyl)amino]-9H-purin-9-yl]-1-naphthalenyl]- (CA INDEX NAME)





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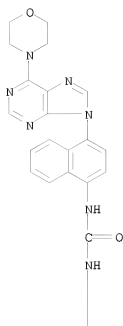


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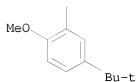
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RN 515843-96-6 CAPLUS  
CN Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-[6-(4-morpholinyl)-9H-purin-9-yl]-1-naphthalenyl]- (CA INDEX NAME)

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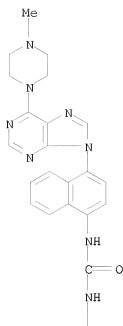


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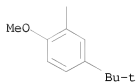


RN 515843-97-7 CAPLUS  
CN Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-[6-(4-methyl-1-piperazinyl)-9H-purin-9-yl]-1-naphthalenyl]- (CA INDEX NAME)

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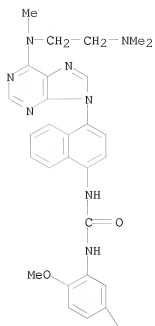


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RN 515843-98-8 CAPLUS  
CN Urea, N-[4-[6-[[2-(dimethylamino)ethyl]methylamino]-9H-purin-9-yl]-1-naphthalenyl]-N'-[5-(1,1-dimethylethyl)-2-methoxyphenyl]- (CA INDEX NAME)

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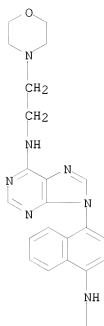


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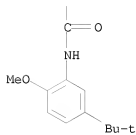
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RN 515843-99-9 CAPLUS  
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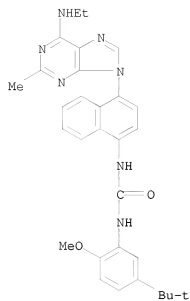
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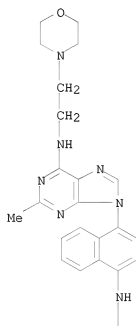
RN 515844-00-5 CAPLUS  
 CN Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-[6-(ethylamino)-2-methyl-9H-purin-9-yl]-1-naphthalenyl]- (CA INDEX NAME)



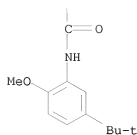
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CN Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-{2-methyl-6-[(2-(4-morpholinyl)ethyl)amino]-9H-purin-9-yl]-1-naphthalenyl]- (CA INDEX NAME)

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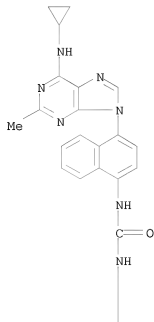


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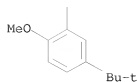


RN 515844-02-7 CAPLUS  
 CN Urea, N-[4-[6-(cyclopropylamino)-2-methyl-9H-purin-9-yl]-1-naphthalenyl]-  
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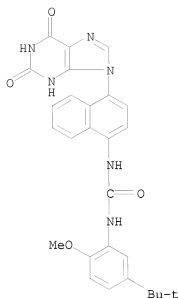
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RN 515844-04-9 CAPLUS  
 CN Urea, N-[5-(1,1-dimethylethyl)-2-methoxyphenyl]-N'-[4-(1,2,3,6-tetrahydro-  
 2,6-dioxo-9H-purin-9-yl)-1-naphthalenyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD  
(11 CITINGS)  
REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1977:478248 CAPLUS

DOCUMENT NUMBER: 87:78248

ORIGINAL REFERENCE NO.: 87:12365a,12368a

TITLE: Quantitative structure-activity studies. Part III.  
Use of van der Waals volume in structure-activity  
studies

AUTHOR(S): Moriguchi, Ikuo; Kanada, Yayoi

CORPORATE SOURCE: Sch. Pharm. Sci., Kitasato Univ., Tokyo, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1977), 25(5),  
926-35

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Several structure-activity data, which had been analyzed using molar  
attraction constant, partition coefficient, connectivity index, and molar  
refraction as a parameter for drug structure, were reexamd. by the use of  
van der Waals volume (VW). These data included in vivo antibacterial  
activity of penicillins, tadpole narcosis with miscellaneous compds.,  
inhibition of neuraminidase by dihydroisoquinolines, fungus toxicity with  
miscellaneous mols., inhibition of xanthine oxidase by phenylguanines, and  
tuberculostatic activity of isoniazid derivs. In all cases, very  
significant correlations were found by regression anal. These findings  
supported the generality of the use of VW to analyze and predict biol.  
activity relating to mol. structure.

IT 20566-66-9 21318-99-0 21864-31-3

21864-34-6 21864-35-7 21864-36-8

21864-38-0 21952-25-0

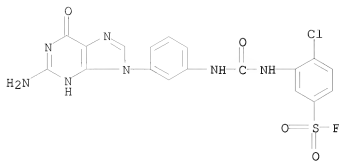
RL: BIOL (Biological study)

(xanthine oxidase inhibition by, van der Waals volume in determination of)

RN 20566-66-9 CAPLUS

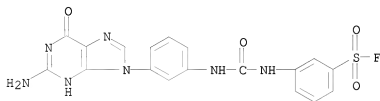
CN Benzenesulfonyl fluoride, 3-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-  
yl)phenyl]amino]carbonyl]amino]-4-chloro- (CA INDEX NAME)





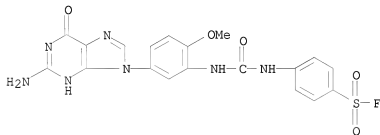
RN 21318-99-0 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]- (CA INDEX NAME)



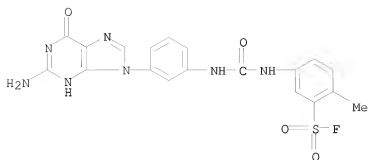
RN 21864-31-3 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[5-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-2-methoxyphenyl]amino]carbonyl]amino]- (CA INDEX NAME)



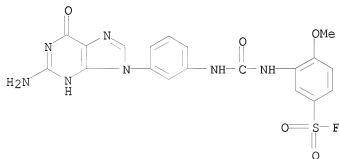
RN 21864-34-6 CAPLUS

CN Benzenesulfonyl fluoride, 5-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-methyl- (CA INDEX NAME)



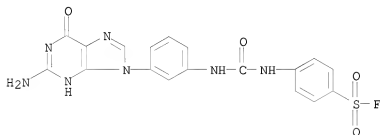
RN 21864-35-7 CAPLUS

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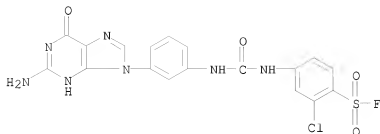
RN 21864-36-8 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]- (CA INDEX NAME)

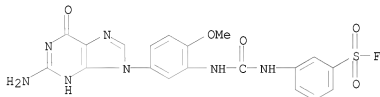


RN 21864-38-0 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-chloro- (CA INDEX NAME)



RN 21952-25-0 CAPLUS  
 CN Benzenesulfonyl fluoride, 3-[[[5-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-2-methoxyphenyl]amino]carbonyl]amino]- (CA INDEX NAME)



OS.CITING REF COUNT: 20 THERE ARE 20 CAPLUS RECORDS THAT CITE THIS RECORD (20 CITINGS)

L5 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1976:38576 CAPLUS

DOCUMENT NUMBER: 84:38576

ORIGINAL REFERENCE NO.: 84:6271a,6274a

TITLE: Correlation analysis of Baker's studies on enzyme inhibition. 1. Guanine deaminase, xanthine oxidase, dihydrofolate reductase, and complement

AUTHOR(S): Silipo, Carlo; Hansch, Corwin

CORPORATE SOURCE: Dep. Chem., Pomona Coll., Claremont, CA, USA

SOURCE: Journal of Medicinal Chemistry (1976), 19(1), 62-71

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Two correlation equations were developed relating inhibitory activity of guanine deaminase [9033-16-3] and xanthine oxidase [9002-17-9] inhibitors to their chemical structure. These equations were based on data obtained by B.R. Baker (1967) using approx.90 inhibitors of these 2 enzyme systems. The importance of indicator variables in correlation anal. of enzymes for drug development was discussed.

IT 20566-66-9 21318-99-0 21864-31-3

21864-34-6 21864-35-7 21864-36-8

21864-38-0 21952-25-0 33873-39-1

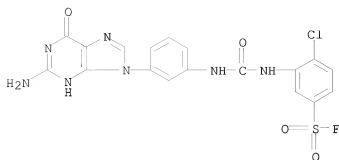
33873-40-4 33873-41-5 33873-42-6

RL: BIOL (Biological study)

(enzyme inhibition by, correlation anal. of)

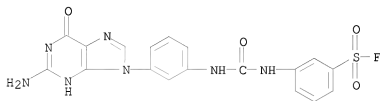
RN 20566-66-9 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-4-chloro- (CA INDEX NAME)



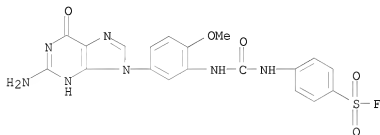
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CN Benzenesulfonyl fluoride, 3-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]- (CA INDEX NAME)



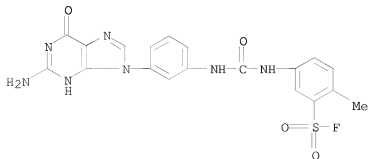
RN 21864-31-3 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[5-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-2-methoxyphenyl]amino]carbonyl]amino]- (CA INDEX NAME)



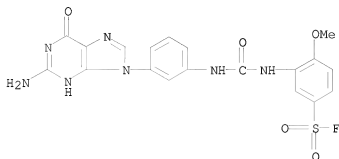
RN 21864-34-6 CAPLUS

CN Benzenesulfonyl fluoride, 5-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-methyl- (CA INDEX NAME)



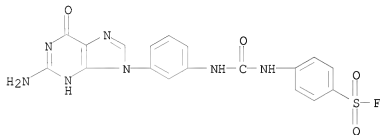
RN 21864-35-7 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-4-methoxy- (CA INDEX NAME)



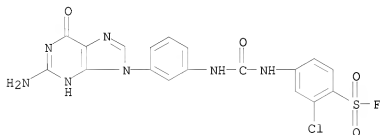
RN 21864-36-8 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]- (CA INDEX NAME)



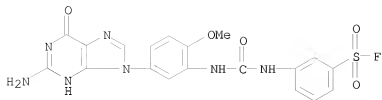
RN 21864-38-0 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-chloro- (CA INDEX NAME)



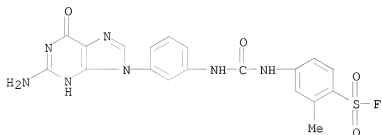
RN 21952-25-0 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[5-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-2-methoxyphenyl]amino]carbonyl]amino]- (CA INDEX NAME)



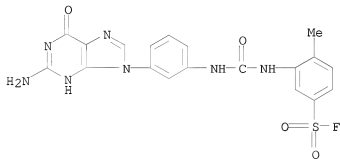
RN 33873-39-1 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-methyl- (CA INDEX NAME)



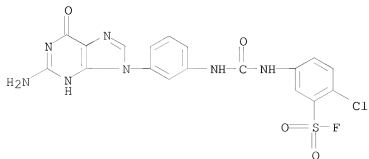
RN 33873-40-4 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-4-methyl- (CA INDEX NAME)

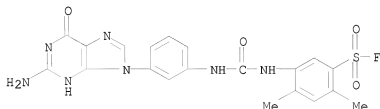


RN 33873-41-5 CAPLUS

CN Benzenesulfonyl fluoride, 5-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-chloro- (CA INDEX NAME)



RN 33873-42-6 CAPLUS  
CN Benzenesulfonyl fluoride, 5-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2,4-dimethyl- (CA INDEX NAME)



OS.CITING REF COUNT: 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)

L5 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2009 ACS on SIN

ACCESSION NUMBER: 1971:529761 CAPLUS

DOCUMENT NUMBER: 75:129761

ORIGINAL REFERENCE NO.: 75:20487a,20490a

TITLE: Irreversible enzyme inhibitors. 185.  
Active-site-directed irreversible inhibitors of guanine deaminase derived from 9-phenylguanine bearing a terminal sulfonyl fluoride. 2

AUTHOR(S): Baker, B. R.; Siebeneick, Hans U.

CORPORATE SOURCE: Dep. Chem., Univ. California, Santa Barbara, CA, USA

SOURCE: Journal of Medicinal Chemistry (1971), 14(9), 802-5

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB Eleven derivs. of 9-phenylguanine bridged from its meta position and 11 derivs. of 9-(p-ethoxyphenyl)guanine bridged from its terminal Me group by carboxamide or ureido bridges to substituted benzenesulfonyl fluorides were synthesized and investigated as irreversible inhibitors of Walker 256 rat tumor guanine deaminase. Four of these compds., 9-[3-(4-chloro-3-fluorosulfonylbenzamido)phenyl]guanine (I), 9-[3-(2,4-dichloro-3-fluorosulfonylbenzamido)phenyl]guanine (II), 9-[3-(3-chloro-4-fluorosulfonylbenzamido)phenyl]guanine (III), and 9-[3-(4-fluorosulfonyl-3-methylbenzamido)phenyl]guanine (IV), gave essentially complete inactivation of the tumor enzyme, but failed to show tissue specificity, since rat liver guanine deaminase was also inactivated by these compds. The 2 acetylamido series were prepared by acylation of 9-(m-aminophenyl)guanine of 9-(p-aminoethoxyphenyl)guanine with the appropriate acid chloride. The 2 phenylureido series were synthesized by condensation of the 2 amines with appropriate O-(p-nitrophenyl)-N-arylcarbamate.

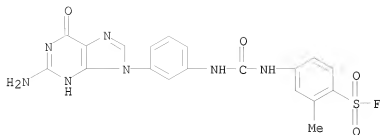
IT 33873-39-1P 33873-40-4P 33873-41-5P

33873-42-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

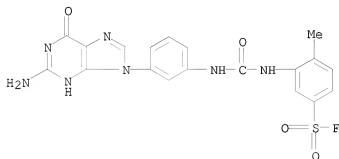
RN 33873-39-1 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-methyl- (CA INDEX NAME)



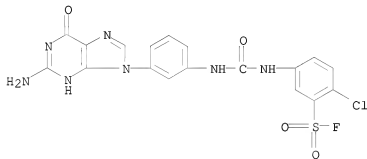
RN 33873-40-4 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-4-methyl- (CA INDEX NAME)



RN 33873-41-5 CAPLUS

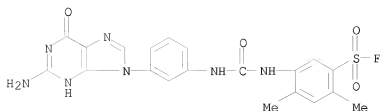
CN Benzenesulfonyl fluoride, 5-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-chloro- (CA INDEX NAME)



RN 33873-42-6 CAPLUS

CN Benzenesulfonyl fluoride, 5-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2,4-dimethyl- (CA INDEX NAME)





OS.CITING REF COUNT: 9 THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD  
(9 CITINGS)

L5 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1969:103224 CAPLUS

DOCUMENT NUMBER: 70:103224

ORIGINAL REFERENCE NO.: 70:19261a,19264a

TITLE: Irreversible enzyme inhibitors. CXLVIII.  
Active-site-directed irreversible inhibitors of  
guanine deaminase derived from p-phenylguanine bearing  
a terminal phenylenesulfonyl fluoride  
Baker, Bernard Randall; Wood, William F.  
CORPORATE SOURCE: Univ. of California, Santa Barbara, CA, USA  
SOURCE: Journal of Medicinal Chemistry (1969), 12(2), 216-20  
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

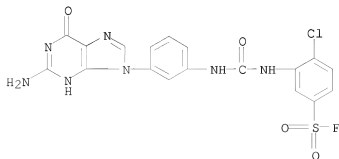
AB Thirty-eight candidate irreversible inhibitors of guanine deaminase  
derived from 9-phenylguanine with a terminal sulfonyl fluoride bridged to  
the meta or para position of the phenyl moiety by an amide or ether  
linkage were evaluated with the enzyme from Walker 256 rat tumor. Three  
of the compds. (I-III) were excellent irreversible inhibitors of this  
enzyme, but also showed no isozyme specificity since these could also  
inactivate the rat liver enzyme. Of the 13 compds. showing moderate  
irreversible inhibition of the Walker 256 enzyme, 4 (IV-VII) showed  
isozyme specificity with no inactivation of the rat liver enzyme.

IT 20566-66-9 21318-99-0 21864-31-3  
21864-34-6 21864-35-7 21864-36-8  
21864-38-0 21952-25-0

RL: BIOL (Biological study)  
(guanine deaminase inhibition by)

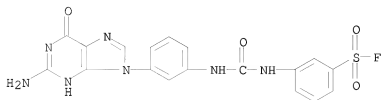
RN 20566-66-9 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-4-chloro- (CA INDEX NAME)



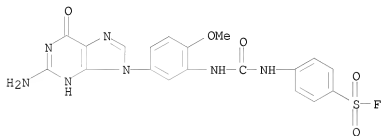
RN 21318-99-0 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]- (CA INDEX NAME)



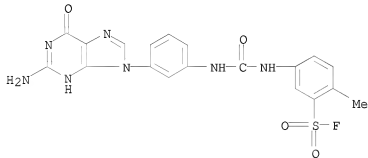
RN 21864-31-3 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[5-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-2-methoxyphenyl]amino]carbonyl]amino]- (CA INDEX NAME)



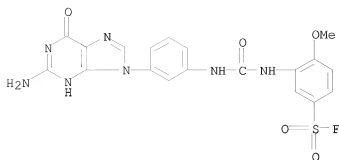
RN 21864-34-6 CAPLUS

CN Benzenesulfonyl fluoride, 5-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-methyl- (CA INDEX NAME)



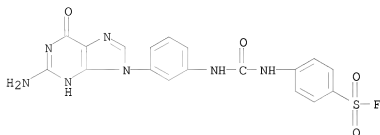
RN 21864-35-7 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-4-methoxy- (CA INDEX NAME)



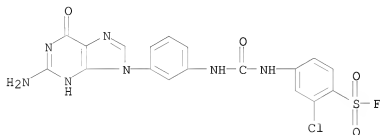
RN 21864-36-8 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]- (CA INDEX NAME)



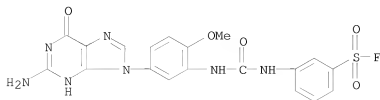
RN 21864-38-0 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-chloro- (CA INDEX NAME)



RN 21952-25-0 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[5-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-2-methoxyphenyl]amino]carbonyl]amino]- (CA INDEX NAME)



OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD  
(6 CITINGS)

L5 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1969:96759 CAPLUS

DOCUMENT NUMBER: 70:96759

ORIGINAL REFERENCE NO.: 70:18085a,18088a

TITLE: Irreversible enzyme inhibitors. CXLVI.  
Active-site-directed irreversible inhibitors of  
xanthine oxidase derived from  
9-(acylamidophenyl)guanines substituted with a  
terminal phenylenesulfonyl fluoride

AUTHOR(S): Baker, Bernard Randall; Wood, William F.

CORPORATE SOURCE: Univ. of California, Santa Barbara, CA, USA

SOURCE: Journal of Medicinal Chemistry (1969), 12(2), 211-14

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Twenty candidate active-site-directed irreversible inhibitors of xanthine oxidase have been synthesized and evaluated. These were derived from m- or p-amino-9-phenylguanine attached to benzenesulfonyl fluoride by a sulfonamide, carboxamide, or urea bridge. Three excellent irreversible inhibitors emerged that at a concentration of 10<sup>-6</sup> to 10<sup>-7</sup> M gave total inactivation of xanthine oxidase with a half-life of 1 min. or less; these were 9-phenylguanines substituted by a p-(p-fluorosulfonylbenzamido), p-(m-fluorosulfonylbenzamido), or m-(p-fluorosulfonylbenzenesulfonamido) moiety.

IT 20566-66-9P 21864-31-3P 21864-34-6P

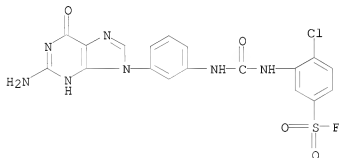
21864-35-7P 21864-36-8P 21864-38-0P

21952-25-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

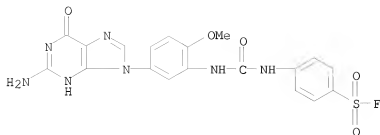
RN 20566-66-9 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-4-chloro- (CA INDEX NAME)



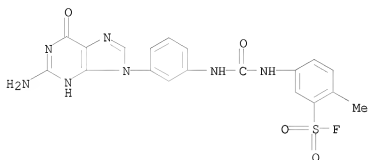
RN 21864-31-3 CAPLUS

CN Benzenesulfonyl fluoride, 4-[[[5-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-2-methoxyphenyl]amino]carbonyl]amino]- (CA INDEX NAME)



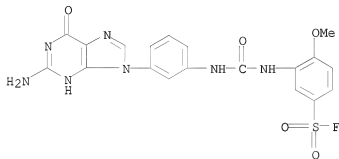
RN 21864-34-6 CAPLUS

CN Benzenesulfonyl fluoride, 5-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-methyl- (CA INDEX NAME)



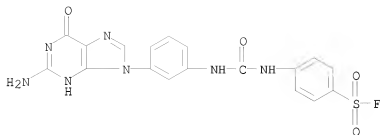
RN 21864-35-7 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-4-methoxy- (CA INDEX NAME)

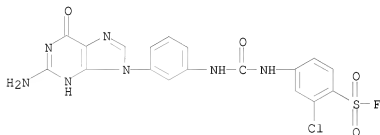


RN 21864-36-8 CAPLUS

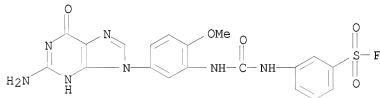
CN Benzenesulfonyl fluoride, 4-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]- (CA INDEX NAME)



RN 21864-38-0 CAPLUS  
 CN Benzenesulfonyl fluoride, 4-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]-2-chloro- (CA INDEX NAME)



RN 21952-25-0 CAPLUS  
 CN Benzenesulfonyl fluoride, 3-[[[5-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-2-methoxyphenyl]amino]carbonyl]amino]- (CA INDEX NAME)



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD  
 (5 CITINGS)

L5 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1968:433164 CAPLUS

DOCUMENT NUMBER: 69:33164

ORIGINAL REFERENCE NO.: 69:6175a,6178a

TITLE: Irreversible enzyme inhibitors. CXXIII. Candidate irreversible inhibitors of guanine deaminase and xanthine oxidase derived from 9-phenylguanine substituted with a terminal sulfonyl fluoride  
 Baker, B. R.; Wood, William F.

AUTHOR(S): Univ. of California, Santa Barbara, CA, USA

CORPORATE SOURCE: Journal of Medicinal Chemistry (1968), 11(4), 650-2

SOURCE: CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 9-[p-(p-Fluorosulfonylbenzamido)phenyl]guanine (I) at 0.7 + 10-6 M

was an excellent active-site-directed irreversible inhibitor of xanthine oxidase, causing 85% inactivation in 1 min. at 37° and 97% in 24 min.; in contrast, I fails to inactivate guanine deaminase at 21 + 10-6M. When the fluorosulfonylbenzamido moiety was moved to the meta position, better reversible inhibitors emerged, but no irreversible inhibition of either xanthine oxidase or guanine deaminase occurred.

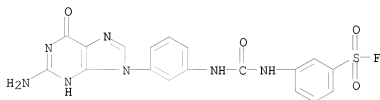
IT 21318-99-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

RN (preparation of and inhibition of guanine deaminase and xanthine oxidase by)

RN 21318-99-0 CAPLUS

CN Benzenesulfonyl fluoride, 3-[[[3-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)phenyl]amino]carbonyl]amino]- (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD  
(2 CITINGS)

=> logoff

ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF

LOGOFF? (Y)/N/HOLD:y

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